Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Dichloromaleic anhydride

Alexander J. Blake *et al.*

Electronic paper
This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Dichloromaleic anhydride

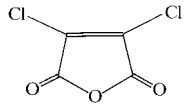
Alexander J. Blake,* Rhiannon M. T. Griffiths, Steven M. Howdle and Claire Wilson

School of Chemistry, The University of Nottingham, University Park, Nottingham NG7 2RD, England
Correspondence e-mail: a.j.blake@nottingham.ac.uk

Received 28 April 2000
Accepted 8 May 2000

Data validation number: IUC0000140

Although molecules of the title compound, 3,4-dichloro-2,5-dihydrofuran-2,5-dione (dichloromaleic anhydride, $C_4Cl_2O_3$), (I), possess approximate non-crystallographic C_{2v} symmetry, the two chlorine substituents deviate from the ring plane. Their deviations are in the same direction, but with values of 0.0356 (17) and 0.0167 (17) Å, they differ significantly in magnitude. The closest intermolecular contact is of 2.888 (2) Å between a carbonyl O atom and the C atom of a carbonyl group, with the O···C direction orthogonal to the C=O bond [O5···C2^{i}=O2^{i} 93.6 (2)°; symmetry code: (i) $\frac{3}{2}-x$, $-\frac{1}{2}+y$, z]. These contacts form infinite chains of molecules running parallel to the crystallographic b direction.



(I)

Experimental

The title compound was crystallized by refluxing with 1*H*,1*H*-perfluoroheptanol.

Crystal data

$C_4Cl_2O_3$
M_r = 166.94
Orthorhombic, *Pbca*
a = 10.6397 (6) Å
b = 8.2558 (5) Å
c = 13.0057 (7) Å
V = 1142.41 (11) Å^3
Z = 8
D_x = 1.941 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5130 reflections
θ = 3.12–28.55°
μ = 1.050 mm^{-1}
T = 150 (2) K
Block, colourless
0.32 × 0.32 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1996)
T_{min} = 0.730, T_{max} = 0.779
7980 measured reflections
1372 independent reflections
1261 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 28.55°
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 17$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.067
S = 1.041
1372 reflections
83 parameters
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.340P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0056 (7)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 1999).

We thank EPSRC (UK) for the award of a diffractometer, the University of Nottingham for a studentship (RMTG) and Dr M. R. Giles for help and advice.

References

Bruker (1996). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SMART Area-Detector Software Package*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT Frame Integration Software*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1999). *PLATON*. University of Utrecht, The Netherlands.